

# Effect of Superconductivity on the Incommensurate Magnetic Response of Cuprate Superconductors

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We explain the effects of superconductivity on the incommensurate magnetic response  $\chi''(\mathbf{q}, \omega)$  observed in inelastic neutron scattering measurements on  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ . We show that a spin-fermion model correctly describes the frequency and momentum dependent changes of  $\chi''$  in the superconducting phase. We find these changes are generic features of an incommensurate spin structure and the d-wave symmetry of the superconducting gap and are thus expected for all cuprates with an incommensurate magnetic response. Our analysis of INS experiments in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  up to optimal doping suggests a Fermi surface which is closed around  $(\pi, \pi)$ .

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The spin excitation spectrum in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  [1–5] in the normal and superconducting state has been intensively studied during the last few years by inelastic neutron scattering (INS) experiments. The normal state spectrum for compounds with  $x > 0.04$  is characterized by peaks in  $\chi''(\mathbf{q}, \omega)$  at incommensurate wave-vectors  $\mathbf{Q}_i = (1 \pm \delta, 1)\pi$  and  $\mathbf{Q}_i = (1, 1 \pm \delta)\pi$  [1,2,5], where  $\delta$  increases with increasing doping. Recent INS experiments in the superconducting state of  $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$  by Mason *et al.* [2] and  $\text{La}_{1.83}\text{Sr}_{0.17}\text{CuO}_4$  by Lake *et al.* [3] show striking momentum and frequency dependent changes in  $\chi''$  upon entering the superconducting state. They find for both compounds that at the incommensurate wave-vector  $\mathbf{Q}_i$ ,  $\chi''$  in the superconducting state is considerably decreased below its normal state value for  $\omega \leq 7$  meV, while it increases for larger frequencies. Moreover, for frequencies in the vicinity of 7 meV, the incommensurate peaks sharpen in the superconducting state, while at higher frequencies the peak widths in the normal and superconducting state are approximately equal.

In this communication, we show that these experimental results are a direct consequence of changes in the quasiparticle damping of an incommensurate spin structure due to the appearance of a d-wave gap in the superconducting state. We demonstrate that the available INS data provide insight into both the symmetry of the order parameter and Fermi surface topology, and show that INS experiments on  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  suggest a closed Fermi surface around  $(\pi, \pi)$  up to optimal doping. We find that comparable changes in  $\chi''$  are to be expected for any cuprate superconductor with an incommensurate spin spectrum. Our approach should thus apply to  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ , in which Tranquada *et al.* [6] and Dai, Mook *et al.* [7,8] find an incommensurate spin structure at low frequencies.

The starting point for our calculations is a spin-fermion model [9] of incommensurate spin-excitations in which the position and width of the overdamped spin mode are determined by its coupling to the planar quasi-particles. The description of the spin excitations as a relaxational

mode is motivated by the fits to NMR [10] and INS [11] experiments in the normal state, and by the INS experimental observation in  $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$  that no dispersing spin mode exists for  $\omega \leq 25$  meV [12], well above the frequency range we consider here.

In a spin-fermion model [9], the spin-wave propagator,  $\chi$ , is given by

$$\chi^{-1} = \chi_0^{-1} - \text{Re } \Pi - i \text{Im } \Pi, \quad (1)$$

where  $\chi_0$  is the bare propagator, and  $\Pi$  is the irreducible particle-hole bubble. The form of the bare propagator in Eq.(1) is model dependent; however  $(\chi_0^{-1} - \text{Re } \Pi)$  may be taken from fits to NMR and INS experiments in the normal state of  $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$  [10,11],

$$\chi_0^{-1} - \text{Re } \Pi = \frac{1 + \xi^2(\mathbf{q} - \mathbf{Q}_i)^2}{\chi_{\mathbf{Q}_i}}, \quad (2)$$

where  $\xi$  is the magnetic correlation length and  $\chi_{\mathbf{Q}_i}$  is the static staggered susceptibility. On combining Eqs.(1) and (2) we obtain

$$\chi''(\mathbf{q}, \omega) = \chi_{\mathbf{Q}_i} \frac{\Gamma(\omega)}{[1 + \xi^2(\mathbf{q} - \mathbf{Q}_i)^2]^2 + \Gamma(\omega)^2}, \quad (3)$$

where  $\Gamma(\omega) = \chi_{\mathbf{Q}_i} \text{Im } \Pi$ .

We thus need to calculate only the imaginary part of  $\Pi$  which describes the damping brought about by the decay of a spin excitation into a particle-hole pair. In the superconducting state we find to lowest order in the spin-fermion coupling  $g_{eff}$  (for  $\omega > 0$ )

$$\begin{aligned} \text{Im } \Pi(\mathbf{q}, \omega) = & \frac{3\pi g_{eff}^2}{8} \sum_{\mathbf{k}} \left( 1 - n_F(E_{\mathbf{k}+\mathbf{q}}) - n_F(E_{\mathbf{k}}) \right) \\ & \times \left[ 1 - \frac{\epsilon_{\mathbf{k}+\mathbf{q}}\epsilon_{\mathbf{k}} + \Delta_{\mathbf{k}+\mathbf{q}}\Delta_{\mathbf{k}}}{E_{\mathbf{k}+\mathbf{q}}E_{\mathbf{k}}} \right] \delta(\omega - E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) \\ & - \left( n_F(E_{\mathbf{k}}) - n_F(E_{\mathbf{k}+\mathbf{q}}) \right) \left[ 1 + \frac{\epsilon_{\mathbf{k}+\mathbf{q}}\epsilon_{\mathbf{k}} + \Delta_{\mathbf{k}+\mathbf{q}}\Delta_{\mathbf{k}}}{E_{\mathbf{k}+\mathbf{q}}E_{\mathbf{k}}} \right] \\ & \times \left\{ \delta(\omega + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) - \delta(\omega - E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{q}}) \right\}, \quad (4) \end{aligned}$$

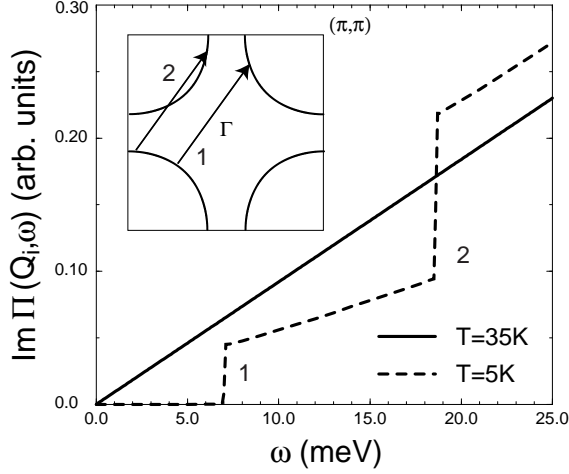


FIG. 1. The spin-damping  $\text{Im } \Pi$  at  $\mathbf{Q}_i$  as a function of frequency in the normal (solid line) and superconducting state (dashed line). Inset: Fermi surface of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  and quasiparticle threshold transitions with wave-vector  $\mathbf{Q}_i$ .

where  $n_F$  is the Fermi function,  $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$  is the fermionic dispersion in the superconducting state,  $\Delta_{\mathbf{k}}$  is the d-wave gap

$$\Delta_{\mathbf{k}}(T) = \Delta_{SC}(T) \frac{\cos(k_x) - \cos(k_y)}{2}, \quad (5)$$

and  $\epsilon_{\mathbf{k}}$  is the tight-binding band for a single-layer system with

$$\epsilon_{\mathbf{k}} = -2t \left( \cos(k_x) + \cos(k_y) \right) - 4t' \cos(k_x) \cos(k_y) - \mu, \quad (6)$$

where  $t, t'$  are the hopping elements between nearest and next-nearest neighbors, respectively, and  $\mu$  is the chemical potential. We determine  $g_{eff}$  by requiring that for a given quasi-particle spectrum,  $\text{Im } \Pi$  reproduces the spin-damping seen at low frequencies in NMR experiments in the normal state (where  $\Delta_{SC} \equiv 0$  in Eq.(4)) just above  $T_c$  and we assume that  $g_{eff}$  does not change in the superconducting state. In what follows, we consider for definiteness  $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$  [11], where a choice of  $t = 300$  meV,  $t' = -0.22t$ , and  $\mu = -0.81t$  yields the best agreement with the experimental data. The superconducting gap,  $\Delta_{SC}(T=0) \approx 10$  meV, was extracted from Raman scattering experiments by Chen *et al.* [13] and the incommensurate wave-vector  $\mathbf{Q}_i$  is at  $\delta = 0.245$  [2,5].

In Fig. 1 we present our results for the spin-damping,  $\text{Im } \Pi$ , at the incommensurate wave-vector  $\mathbf{Q}_i$ . Due to the incommensurate spin-structure one obtains four decay channels for the spin excitations at  $\mathbf{Q}_i$ ; the two channels within the first Brillouin zone are shown in the inset of Fig. 1. In the normal state all four channels can be excited in the low frequency limit, and one finds a linear in frequency dependence of the spin damping. In the superconducting state, the channels split

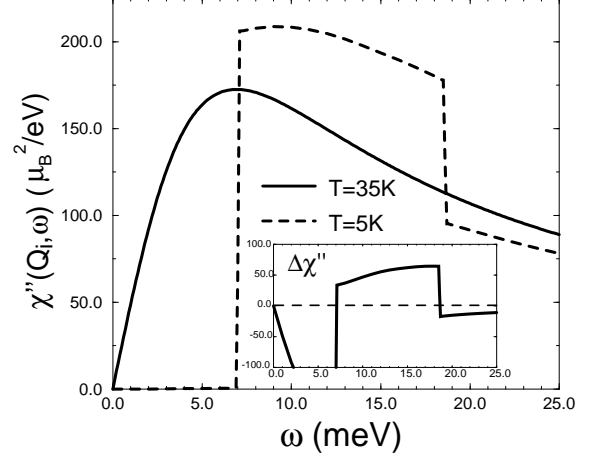


FIG. 2.  $\chi''(\mathbf{Q}_i, \omega)$  in the normal (solid line) and superconducting state (dashed line). Inset:  $\Delta\chi''(\omega) = \chi''_S(\mathbf{Q}_i, \omega) - \chi''_N(\mathbf{Q}_i, \omega)$ .

into two pairs with degenerate finite threshold energies which are determined by the momentum dependence of the order parameter and the shape of the Fermi surface. The frequency position of the thresholds is specified by  $\omega_c^{(1,2)} = |\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{Q}_i}|$ , where  $\mathbf{k}$  and  $\mathbf{k}+\mathbf{Q}_i$  both lie on the Fermi surface, as shown in the inset of Fig. 1. A comparison of the threshold energies thus provides insight into the symmetry of the order parameter, and in particular, is sensitive to its deviation from a pure d-wave symmetry. For the band parameters we have chosen, there are two distinct threshold energies,  $\omega_c^{(1)} = 0.70\Delta_{SC}$  for quasiparticle excitations close to the nodes of the superconducting gap (excitation 1), and  $\omega_c^{(2)} = 1.86\Delta_{SC}$  for excitations close to  $(0, \pi)$  and  $(\pi, 0)$  (excitation 2). At  $T = 0$ , no quasi-particle excitations below  $\omega_c^{(1)}$  can be excited, and the spin-damping vanishes. Both steps in  $\text{Im } \Pi$  will, via the Kramers-Kronig relation, lead to a logarithmic divergence in  $\text{Re } \Pi$ . This is neglected in Eq.(2), since fermion lifetime effects as found, e.g., in strong coupling scenarios [14], smooth out the sharp step in  $\text{Im } \Pi$  and thus eliminates the divergence in  $\text{Re } \Pi$ .

In Fig. 2 we present our results for the normal and superconducting state intensity  $\chi''_N$  and  $\chi''_S$ . Since in the normal state  $\text{Im } \Pi \sim \omega$ , we find  $\chi''_N \sim \omega$  for small frequencies, followed by a maximum for  $\Gamma(\omega) = 1$  (which within experimental errors occurs at approx. 7 meV [2]), and by  $\chi''_N \sim 1/\omega$  at high frequencies. On the other hand,  $\chi''_S$  is characterized by jumps at  $\omega_c^{(1,2)}$ , which reflect the behavior of  $\text{Im } \Pi$ ; an enhancement over the normal state intensity is found for the frequency range between the two jumps. This enhancement follows straightforwardly from Eq.(3) as long as the condition  $1/\Gamma_N(\omega) \leq \Gamma_S(\omega) \leq \Gamma_N(\omega)$  (for  $\chi''_S/\chi''_N = 1$ ) is satisfied. From Fig. 1 we find that this condition is met in a finite frequency region, leading to two crossings of  $\chi''_N$  and  $\chi''_S$ . The loca-

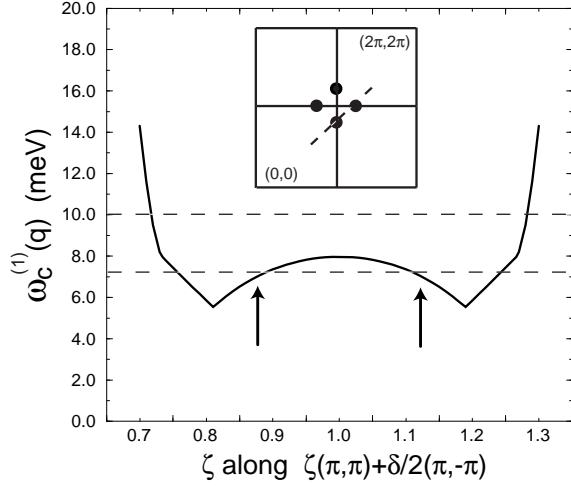


FIG. 3.  $\omega_c^{(1)}(\mathbf{q})$  along the path shown in the inset. The arrows indicate the position of the incommensurate peaks at  $\zeta = 1 \pm \delta/2 = 0.88(1.12)$ . Inset: momentum space path with  $\mathbf{q} = \zeta(\pi, \pi) + \delta/2(\pi, -\pi)$ .

tion in frequency space of the lower crossing depends not only on  $\omega_c^{(1)}$ , but also on the ratio of the peak strengths,  $\chi_{\mathbf{Q}_i}^S/\chi_{\mathbf{Q}_i}^N$ , or what is equivalent, to the ratio of the corresponding correlation lengths, since  $\chi_{\mathbf{Q}_i} = \alpha\xi^2$ , where  $\alpha$  is a temperature independent scale factor. On comparing our results with the experimental results [2], which show a lower crossing at  $\approx 7$  meV, a resolution limited decrease of  $\chi_S''$  below this crossing [3] and a slightly enhanced  $\chi_{\mathbf{Q}_i}$  in the superconducting state, we conclude that a ratio  $\chi_{\mathbf{Q}_i}^S/\chi_{\mathbf{Q}_i}^N \approx 1.2$  provides a reasonable fit to experiment. The corresponding value of  $\Delta\chi'' = \chi_S'' - \chi_N''$  is presented in the inset of Fig. 2.

We turn next to changes in the momentum dependence of  $\chi''$  at fixed frequency as one goes from the normal to the superconducting state. These changes arise from the momentum dependence of  $\omega_c^{(1)}(\mathbf{q})$  in the vicinity of  $\mathbf{Q}_i$ . In Fig. 3 we plot  $\omega_c^{(1)}(\mathbf{q})$  for the momentum space path considered in Ref. [2],  $\mathbf{q} = \zeta(\pi, \pi) + \delta/2(\pi, -\pi)$  (see inset). A momentum dependence of  $\omega_c^{(1)}(\mathbf{q})$  which agrees with the experimentally observed threshold frequency for non-zero  $\chi_S''$  [3,12], gives rise to several interesting effects. First, since the minimum  $\omega_{min} = 5.5$  meV in  $\omega_c^{(1)}(\mathbf{q})$  does not occur at the incommensurate wave-vectors  $\mathbf{Q}_i$ , a non-zero  $\chi_S''$  (at  $\omega \geq \omega_{min}$ ) first appears at wavevectors slightly removed from  $\mathbf{Q}_i$ . Second, as the frequency increases above  $\omega_{min}$ , the region in momentum space in which  $\chi_S''$  is finite widens, and as a result more of the incommensurate peak, centered at  $\mathbf{Q}_i$ , becomes "visible". One thus obtains not only an increase of the peak intensity with increasing frequency, but also a shift of the peak maximum towards  $\mathbf{Q}_i$ , in full agreement with the experimental data [3,12]. It follows from Fig. 3 that this effect should vanish for frequencies larger than the local

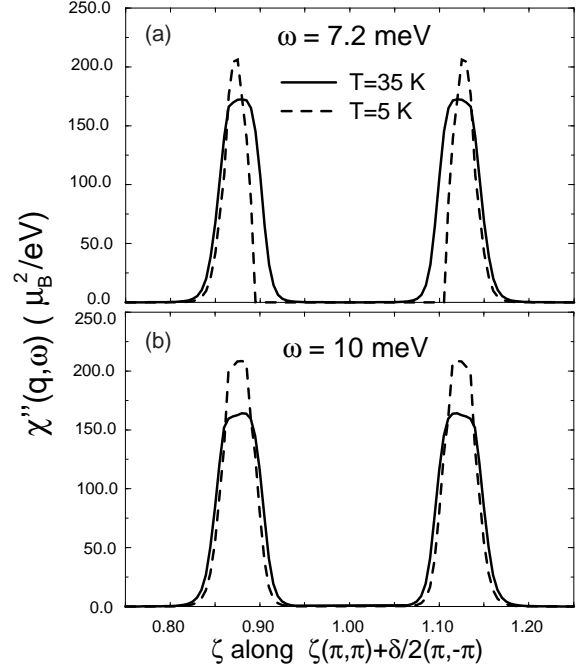


FIG. 4.  $\chi''(\mathbf{q}, \omega)$  in the normal (solid line) and superconducting state (dashed line) for fixed frequency (a)  $\omega = 7.2$  meV and (b)  $\omega = 10.0$  meV, along the same momentum space path as in Fig. 3.

maximum of  $\omega_c^{(1)}(\mathbf{q})$  at  $\zeta = 1$ ,  $\omega_{max}^{loc} = 8$  meV.

In Fig. 4 we plot the normal and superconducting  $\chi''$  for  $\omega = 7.2$  meV and  $\omega = 10.0$  meV, corresponding to the lower and upper dashed curves in Fig. 3, respectively. Since the frequency in Fig. 4a is between  $\omega_c^{(1)} \equiv \omega_c^{(1)}(\mathbf{Q}_i)$  and  $\omega_{max}^{loc}$ ,  $\chi_S''$  increases compared to the normal state result, while the width of the peak in the superconducting state is narrower than that in the normal state and the maximum of the peak intensity is shifted away from  $\mathbf{Q}_i$ . In contrast, for  $\omega = 10.0$  meV  $> \omega_{max}^{loc}$  (Fig. 4b) the peak is centered around  $\mathbf{Q}_i$  and the peak widths in the normal and superconducting state are approximately equal. All of these results, i.e., narrow peaks in the vicinity of  $\omega_c^{(1)}(\mathbf{Q}_i)$  as well as the increase in peak width and the shift towards  $\mathbf{Q}_i$  with increasing frequency agree with the experimental findings of Ref. [2,3].

An additional interesting effect appears as one moves away from  $\mathbf{Q}_i$ . Due to the symmetry of the Fermi surface, the double-degeneracy of the threshold frequencies is lifted for  $\mathbf{q} \neq \mathbf{Q}_i$ . While the frequency positions of the two upper thresholds stay close, the separation between the two lower threshold energies increases rapidly with distance from  $\mathbf{Q}_i$ , e.g., for  $\zeta = 0.89$  the lower thresholds are located at 7.1 meV and 10.0 meV, resulting in two sharp increases of  $\chi_S''(\omega)$  at these energies. We thus predict that as one moves away from  $\mathbf{Q}_i$ ,  $\chi_S''(\omega)$  should not only decrease in intensity, but also acquire some new structure due to additional frequency thresholds. Some

support for this prediction comes from our results for  $\zeta = 0.94$ , where we obtain two sharp increases of  $\chi_S''(\omega)$  at 7.7 meV and 16 meV, with an almost constant intensity in between, in qualitative agreement with the experimental data [3]. However, due to the decrease in the signal-to-noise ratio as one moves away from  $\mathbf{Q}_i$  a better experimental resolution is required to allow a quantitative comparison with our predictions.

Within our scenario, the available INS data also provide insight into the Fermi surface topology of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ . While we find that  $\omega_c^{(2)}$  is robust against changes in the bandstructure parameters,  $\omega_c^{(1)}$  depends very sensitively on the Fermi surface topology, i.e.,  $t'$ , due to the strong momentum dependence of the superconducting gap in the vicinity of the nodes. The location of  $\omega_c^{(1)}$  is therefore a sensitive probe of the form of the Fermi surface and can be used to extract  $t'$  from the experimental data. Though the limited experimental resolution leaves some uncertainty in  $\omega_c^{(1)}$ , and thus in  $t'$ , we find that the INS data provide a lower bound for  $t'$ . Within our scenario for the superconducting state, particle-particle excitations in the vicinity of the nodes become impossible for  $|t'| < 0.2t$ , hence  $\chi_S''(\omega)$  would vanish for *all* frequencies below  $\omega_c^{(2)}$ , in contradiction to the experimental results. Moreover, assuming a weak doping dependence of  $t'$ , this lower bound  $|t'| \geq 0.2t$  yields a Fermi surface of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  which is closed around  $(\pi, \pi)$  up to optimal doping. The Fermi surface thus possesses the same topology as the one in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ ; this offers a possible explanation for the occurrence of incommensurate peaks in the spin spectrum along the same direction in momentum space in the latter materials [6–8]. Two additional constraints for the form of the Fermi surface come from the location of the minimum in  $\omega_c^{(1)}(\mathbf{q})$  (see Fig. 3) and the appearance of additional structure in  $\chi_S''(\omega)$  at  $\mathbf{q} \neq \mathbf{Q}_i$ , which both strongly depend on  $t'$ .

It follows from the above analysis that  $\omega_c^{(1)}(\mathbf{Q}_i)$  is sensitive to the extent of incommensuration in the spin spectrum. Using the doping dependence of  $\delta$  in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  found by Yamada *et al.* [5] we obtain for  $x = 0.1$  ( $\delta = 0.2$ ),  $\omega_c^{(1)}(\mathbf{Q}_i) = 0.93\Delta_{sc}$ , while for  $x = 0.08$  ( $\delta = 0.16$ ) we find  $\omega_c^{(1)}(\mathbf{Q}_i) = 1.14\Delta_{sc}$ . We thus predict that the ratio  $\omega_c^{(1)}(\mathbf{Q}_i)/\Delta_{sc}$  should increase with decreasing doping.

Though the details of the effects which we discussed are sensitive to material specific parameters, e.g., Fermi surface topology, extent of  $\delta$ , their experimental observation within our scenario only depends on two criteria: the existence of an incommensurate spin structure and a d-wave gap in the superconducting state; we thus predict comparable changes in  $\chi_S''$  for all cuprate superconductors in which these criteria are met.

Finally, it was recently pointed out that the formation of charged stripes, which, it was suggested could be the origin of the incommensurate spin ordering, would give

rise to a substantially "smeared out" Fermi surface [15]. This in turn should lead to a much softer increase of  $\chi_S''(\mathbf{Q}_i)$  above  $\omega_c^{(1)}$ , in contrast to the actually very sharp and resolution limited increase observed by Lake *et al.* [3,12].

In summary, we find that the frequency and momentum dependent changes of  $\chi_S''$  in the superconducting state are a direct consequence of changes in the quasi-particle spectrum due to the appearance of a d-wave gap. We show that the available INS data also constrain the Fermi surface topology, and suggest a Fermi surface in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  which is closed around  $(\pi, \pi)$  up to optimal doping. We predict that  $\chi_S''(\omega)$  will possess additional threshold energies away from  $\mathbf{Q}_i$ , and that the ratio  $\omega_c^{(1)}(\mathbf{Q}_i)/\Delta_{sc}$  will increase with decreasing doping. Improved experimental resolution will make it possible to test our predictions. Finally, we expect to find comparable changes in  $\chi_S''$  in all cuprate superconductors with incommensurate spin-structure.

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